

Review Form 3

Journal Name:	<a href="#">International Journal of Biochemistry Research &amp; Review</a>
Manuscript Number:	Ms_IJBCRR_130416
Title of the Manuscript:	Computer-aided drug design of small-molecule compounds targeting TIM-3 for cancer immunotherapy
Type of the Article	Original Research Article

PART 1: Comments

	Reviewer's comment	Author's Feedback <i>(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)</i>
Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.	The expensive, tedious, and laborious pursuit of drugs for a particular disease is greatly addressed by using CADD methods. The surveillance of potential drug candidates can be done without the hassle of wet laboratory experiments. Investigation of compounds and interaction with the target molecule can be extensively explored with these kinds of studies.	This manuscript emphasizes the advantages of computational drug discovery (CADD) in addressing challenges like cost, time, and labor in traditional drug development. By leveraging in silico methods such as molecular docking and dynamics simulations, we provide a comprehensive analysis of potential small-molecule inhibitors targeting TIM-3, an emerging immune checkpoint. The study also underscores the broader implications of CADD in reducing experimental workload while delivering insightful preliminary data for subsequent laboratory validation.
Is the title of the article suitable? (If not please suggest an alternative title)	YQG-like compounds can be used instead of “small-molecule compounds” on the title or a different wording that can indicate the limitation of surveying compounds similar to TIM-3 inhibitor.	The title has been revised for clarity and specificity to better reflect the study's focus on YQG-like compounds.
Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here.	Place and duration of the study can be mentioned under the Methods. TIM-3 can be defined in the Abstract part.	Done
Is the manuscript scientifically, correct? Please write here.	The manuscript is scientifically sound.	Thank you
Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.	The author can cite/mention the programs or applications used where the images are generated in Figure titles.	Thank you. We have updated our methods section to include the visualizer we used for depicting the protein-ligand in 2D and 3D style (see the end of section 2.2 of the revised manuscript)

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<b>Is the language/English quality of the article suitable for scholarly communications?</b>	The language quality is fine, however, please ensure that the manuscript is free of any grammatical and spelling errors. It is also suggested to remove the use of word “renowned” in Methodology part that described the programs/applications used.	The manuscript has been thoroughly reviewed for grammatical and spelling errors, and the word "renowned" has been removed to maintain a scholarly tone.
<b><u>Optional/General</u></b> comments	<b>In the Introduction, it was mentioned that the study aimed to investigate the therapeutic potential of targeting TIM-3. However, there was no method used to answer this objective.</b>  <b>Druglikeness can also be included in the study.</b>	The manuscript now includes a discussion of the therapeutic implications of the identified compounds, aligning with the stated aim in the Introduction. Additionally, the molecular docking and dynamics results are explicitly linked to their potential therapeutic relevance.  For Drug-likeness, we believe the compounds are pharmacophores of YQG compound, which suggest they are likely to be a good compounds in terms of their drug-likeness.

**PART 2:**

	<b>Reviewer’s comment</b>	<b>Author’s comment</b> <i>(if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)</i>
<b>Are there ethical issues in this manuscript?</b>	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	